LOS ALAMOS NATIONAL LABORATORY

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

351. **ACTINIDE PROCESSING DEVELOPMENT**
$1,350,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: R. L. Gutierrez, (505) 665-3919

The aim of this project is the development and characterization of fabrication processes and the study of new processing technologies for plutonium. Research involves casting, thermomechanical working, and stability studies. Measurements of resistivity, thermal expansion, magnetic susceptibility, and formability are made to evaluate fabrication processes and alloy stability.

Keywords: Radioactive Materials, Plutonium Alloys, Ductility, Thermal Expansion, Electrical Resistivity, Stability

352. **PLUTONIUM OXIDE REDUCTION**
$150,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: K. Axler, (505) 667-4045

The thermodynamics of interactions among the components used in the pyrochemical processing of plutonium are determined along with the relevant phase relations.

Keywords: Radioactive Materials, Plutonium, Thermodynamics, Phase Diagrams, Direct Oxide Reduction, Electrorefining, Molten Salt Extraction

353. **LOW DENSITY MICROCELLULAR PLASTIC FOAMS**
$200,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: P. Apen, (505) 667-6887

Microstructural polyolefin foams with densities between 0.01 g/cc and 0.2 g/cc are manufactured by a nonconventional foaming process. Foams are both open and closed celled and have large surface areas. This process is being expanded to other polymeric materials for a wide variety of applications. Foams have cell sizes from 25μm down to the 1μm range, depending on the process. Composite foams are being produced with submicron cell sizes while maintaining structural properties.

Keywords: Foams, Polyolefins, Polyurethanes, Silicones, Polyesters

354. **PHYSICAL VAPOR DEPOSITION AND SURFACE ANALYSIS**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: M. Scott, (505) 667-7557

Physical vapor deposition, one electron beam sputtering, and dual ion beam sputtering are employed to produce materials for structural applications, corrosion resistance, optical properties, and thin film transducers. Materials being developed include doped, *in situ* laminates of aluminum and Al_xO_y having high strength and smooth surface finish. Also included are ion assisted deposition and ion sputtering onto various substrates for corrosion resistance to gases and liquid plutonium, reflective and anti-reflective coatings for infrared, visible, ultraviolet and X-ray wavelengths. Novel photocathodes are being made and evaluated by these processes.

Keywords: Coatings and Films, Physical Vapor Deposition, Sputtering, Ion Plating, Corrosion, Nondestructive Evaluation

355. **CHEMICAL VAPOR DEPOSITION (CVD) COATINGS**
$150,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contacts: J. R. Laia and M. Trkula, (505) 667-0591

Chemical vapor deposition (CVD) techniques are used to deposit thin-film and bulk coatings of a wide variety of elements and compounds. Coatings are deposited by the following techniques: conventional flow-by, fluidized-bed, plasma-assisted, and chemical vapor infiltration. To support and enhance our basic CVD program, efforts are underway to study the fundamental nature of the CVD process, including *in situ* diagnostics in the gas phase just above the substrate and modeling efforts to predict gas flows, reactor design, and chemical behavior within the CVD systems. Another collaborative effort at Los Alamos is attempting to synthesize organometallic precursors to deposit coatings at temperatures <300°C. Substrates coated by the CVD technique range from particles 2.0 μm diameter to infiltrations of fabrics a square meter in area.

Applications include nuclear and conventional weapons, space nuclear reactor systems (fuels and structural

components), inertial confinement fusion program, high temperature engine and structural components for advanced high-performance aircraft, hard/wear resistant coatings (tribological), corrosion resistant coatings, coatings of complex geometries, near-net-shape fabrication, heat-pipe structures, precision CVD of ultra-thin, freestanding shapes.

Keywords: Chemical Vapor Deposition, Coatings (metal and ceramic)

356. **POLYMERS AND ADHESIVES**
$430,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: D. A. Hemphill, (505) 667-8335

The objective of this project is to identify potential weapons engineering and physics applications for plastic and composite materials, select or develop appropriate materials, develop low cost fabrication techniques compatible with Integrated Contractor production capabilities, and characterize promising materials on a timely basis to provide optimum material choices for new weapons designs. Material or process development projects include: highly filled polymers, composite structural and spring components, cushioning materials, and high-explosive compatible adhesives, potting materials. This work will be compatible with all current and future ES&H guidelines.

Keywords: Adhesives, Composites, Plastics, Polymers, Weapons Design, Weapons Engineering, Integrated Contractors

357. **TRITIATED MATERIALS**
$175,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: J. R. Bartlit, (505) 667-5419

Advanced research and development efforts are focused on tritiated materials for tritium storage. New methods for preparing, fabricating, and containing such compounds are under investigation. We are also using laser-Raman techniques for *in situ* measurements of hydrogen-deuterium-tritium gas mixtures.

Keywords: Tritium, Tritiated Materials, Radioactive Materials

358. **SALT FABRICATION**
$800,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: D. Carstens, (505) 667-5849

Development and evaluation of new fabrication and containment processes for LiH and LiD. This includes preparation of device parts for WTS tests. Research topics include development of hot pressing, machining techniques for salt compacts.

Keywords: Tritium, Hydrides, Machining, Radioactive Materials, Near-Net-Shape Processing

359. **SLIP CASTING OF CERAMICS**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: D. S. Phillips, (505) 667-5128

We are slip casting many ceramics including alumina, zirconia-toughened alumina (ZTA), and magnesia. The technology uses colloidal chemistry and powder characterization techniques, along with materials engineering. Considerable progress was made in the development of ZTA ceramic alloys with a superior microstructure and improved thermal shock resistance. The scope of work has expanded to include frits and insulation materials, as well as dense crucibles.

Keywords: Ceramics, Microstructure, Strength, Transformation Toughened Ceramics, Thermal Shock

360. **PLASMA-FLAME SPRAYING TECHNOLOGY**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: R. Castro, (505) 667-5191

Free-standing shapes and metallic and ceramic coatings are fabricated by plasma spraying. Materials examined recently include Be, ^{238}U, $MoSi_2$ and ZrO_2. Applications include: radiochemical detectors; temperature-, oxidation-, and corrosion-resistant coatings; and electrically insulating coatings.

Keywords: Coatings, Metals, Ceramics, Plasma-Flame Spraying, High Temperature Service, Surface Characterization and Treatment

361. **RAPID SOLIDIFICATION TECHNOLOGY**
$500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
P. Stanek, (505) 667-6914

RSR technologies such as melt spinning, splat cooling, and rapid solidification plasma spraying, are being developed to evaluate a range of RSR alloys, intermetallics and composites for defense and energy applications. Activities include alloy development, microstructural analysis, mechanical and physical properties testing, process development and modeling.

Keywords: Rapid Solidification, Low Pressure Plasma, Alloy Development, Composites, Intermetallics

362. **BULK CERAMIC PROCESSING**
$250,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
J. D. Katz, (505) 665-1424

Cold pressing and cold isostatic pressing, followed by sintering, are used to produce ceramic and metal components for various physics experiments and for plutonium processing. Materials fabricated include alumina, magnesia and boron.

In addition, a collaborative effort was established with the University of New Mexico Center for Micro-Engineered Ceramics to investigate the effect of 2.45 GHz microwave energy on the diffusion of cations in ceramic oxides. This research consists of both a theoretical and experimental component. The results have shown that although microwave enhanced diffusion of chromium in alumina does not exist, microwave sintering has been found to be a very effective engineering tool for densifying even large alumina ceramics.

Finally, considerable effort was devoted to developing methods for sintering, rather than hot pressing, boron carbide to achieve high density. This work involves a collaboration with the A.W.E. in the United Kingdom.

Keywords: Ceramics, Sintering, Microwave Sintering, Cold Pressing

363. **SYNTHESIS OF CERAMIC COATINGS**
$150,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
C. P. Scherer, (505) 665-3202

The objective of this effort is to synthesize ceramic films for liquid metal containment. One approach entails the use of organic and aqueous solvents to deposit erbia films, which are subsequently heat treated to densification. The second approach involves the *in situ* conversion of a metal surface to a nitride by precise heating in a nitrogen environment.

Keywords: Ceramic Coatings, Sol Gel, Nitration

MATERIALS STRUCTURE OR COMPOSITION

364. **ACTINIDE SURFACE PROPERTIES**
$700,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
J. M. Haschke, (505) 665-3342

Characterization of actinide metal, alloy and compound surfaces using the techniques of X-ray photoelectron spectroscopy, Auger analysis, ellipsometry and Fourier-transform infrared spectroscopy. Surface reactions, chemisorption, attack by hydrogen, and the nature of associated catalytic processes are being studied.

Keywords: Actinides, Hydrides, Surface Characterization and Treatment, Hydrogen Effects, Radioactive Materials

365. **NEUTRON DIFFRACTION OF PU AND PU ALLOYS AND OTHER ACTINIDES**
$237,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
A. C. Lawson, (505) 667-8844

Physical structure and properties of plutonium are being studied by pulsed neutron diffraction at the Manuel Lujan, Jr., Neutron Scattering Center (Los Alamos) and the Intense Pulsed Neutron Source (Argonne). A time-of-flight technique is used to measure diffraction at cryogenic and elevated temperatures.

Keywords: Alloys, Radioactive Materials, Transformation, Microstructure

366. **SURFACE, MATERIAL AND ANALYTICAL STUDIES**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
W. C. Danen, (505) 667-4686

Studies are underway in four key areas: surface and interfacial structures and properties, explosives dynamics, laser-based isotopic analysis, and metastable energetic materials. Current investigations in surface and interfacial studies include: surface modification, HTSC composition and structure, and the use of MeV ion beams. In explosives chemistry, we are using real-time optical- and mass-spectral methods to probe the early-time dynamics of detonation. Analytical studies have centered on the use of resonance ionization mass spectrometry to eliminate isobaric interferences in the measurement of high-dynamic range isotope ratio measurements. We continue to study the synthesis and characterization of a new class of high energy density materials consisting of atomically-thin multilayered composite materials.

Keywords: Surface, Explosives, Interfaces, Composite Materials

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

367. **MECHANICAL PROPERTIES OF PLUTONIUM AND ITS ALLOYS**
$450,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
R. L. Gutierrez, (505) 665-3919

The mechanical properties of plutonium and its alloys are related to the pre-test and post-test microstructures of the materials using optical and electron microscopy and X-ray, electron and neutron diffraction.

Keywords: Alloys, Radioactive Materials, Microstructures, Strength, Transformation

368. **PHASE TRANSFORMATIONS IN PU AND PU ALLOYS**
$450,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
R. L. Gutierrez, (505) 665-3919

Mechanisms and crystallography of thermally and mechanically induced allotropic transformations are studied with differential scanning calorimetry, optical and electron microscopy and electron and X-ray diffraction.

Keywords: Alloys, Radioactive Materials, Microstructure, Transformations

369. **PLUTONIUM SHOCK DEFORMATION**
$350,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
M. J. Reisfeld, (505) 667-8485

Plutonium and actinide alloys are subjected to shock deformation, recovered without further damage and examined to determine how the shock affected their microstructures and mechanical properties.

Keywords: Radioactive Materials, Plutonium Alloys, Microstructure, Strength

370. **NON-DESTRUCTIVE EVALUATION**
$550,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
Thomas Claytor, (505) 667-1973

Development of Nondestructive Evaluation Technology that produces quantitative estimates of material properties. Use of tomographic techniques to enhance radiographic inspection. Flash, cine-radiography, high speed video recorded optical and X-ray diagnostics of dynamic and ultra-fast events. Real-time radiography. Image enhancement of output results from all techniques. Development of ultrasonic inspection techniques.

Keywords: Nondestructive Evaluation, Radiography, Ultrasonic Microscopy, Tomography, Cine Radiography, Bonding Processes, Real-Time Radiography, Image Enhancement

371. **POWDER CHARACTERIZATION**
$50,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact:
G. J. Vogt, (505) 667-5813

Synthesis and processing of ceramic or metal powders depends critically on the physical characterization of the starting powders being used. Typical starting powders include commercial powders of thoria, magnesia, alumina, tungsten, copper, tungsten carbide, and boron carbide. In the past year, considerable effort has been expended on characterizing palladium alloy powders. Physical properties of interest include particle size and distribution, surface

area, bulk and packed densities, morphology, pore size and distribution, and zeta potential. The crystalline-phase composition of the starting powders and processed powders can be determined by X-ray diffraction.

Keywords: Ceramic Powder, Metal Powder, Particle Size, Superconducting Powder, X-ray Diffraction, Surface Area

372. **SHOCK DEFORMATION IN ACTINIDE MATERIALS**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: R. L. Gutierrez, (505) 665-3919

Measurement of shock-wave profiles in uranium, plutonium, and plutonium alloys. Use of soft-shock recovery test to examine the microstructural changes occurring during shock deformation. Measurement of spall strength in actinide materials and examination of fracture surfaces.

Keywords: Actinides, Shock Deformation, Microstructure, Spall Strength

373. **DYNAMIC MECHANICAL PROPERTIES OF WEAPONS MATERIALS**
$350,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: G. Gray, (505) 667-5452

Measurements of dynamic stress-strain and fracture behavior of materials used for nuclear weapons. Development of plastic constitutive relations.

Keywords: Dynamic, Strength, Fracture, Microstructure

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

374. **TARGET FABRICATION**
$1,500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contact No. W-7405-ENG-36) Contact: L. Foreman, (505) 667-1846
LLNL Contact: W. Hatcher, (510) 422-1100
General Atomics Contact: Ken Schultz, (619) 455-4304

ICF/AGEX targets are fabricated using PVD, CVD, precision micromachining, and polymer chemistry techniques. After the parts are fabricated, the components are assembled using a variety of techniques. These targets are used to provide laser materials interactions data for the inertial confinement fusion community.

Keywords: Inertial Fusion, Target Fabrication

375. **FILAMENT WINDER**
$100,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: B. Benicewicz, (505) 665-0101

The Entec filament winder in MST-7 Plastics is a 4-axis computer-programmed machine with a winding envelope extending up to 4 feet in diameter and 10 feet in length. It is being utilized to wind circumferential or helical cylinders, cones, spheres, and closed-end vessels from a variety of fibers including glass, kevlar, carbon, tungsten, and aluminum oxide. The applications cover a host of programs from within the Laboratory as well as from outside agencies.

Keywords: Filament Winding, Composites

376. **HIGH ENERGY DENSITY WELDING IN HAZARDOUS ENVIRONMENTS**
$800,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: G. Lewis, (505) 667-9663

High power Nd/YAG lasers combined with fiber optic beam delivery systems have been evaluated for welding applications in hazardous environments. Applications include the manufacture of nuclear weapons components and nuclear power reactor repair. High quality structural welds have been achieved without exposing the operators or the welding power supplies to the hazardous environment.

Keywords: Laser Welding, Fiber Optic Beam Delivery, Hazardous Environments, Nuclear Applications

377. **URANIUM SCRAP CONVERSION AND RECOVERY**
$1,500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LANL (Contract No. W-7405-ENG-36) Contact: Dan Knobeloch, (505) 667-4417

Maintain and develop technologies for conversion and recovery of uranium scrap. Maintain and upgrade facilities for processing enriched uranium and managing uranium inventories.

Keywords: Uranium, Uranium Scrap, Enriched Uranium, Recovery, Processing, Inventories

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

378. **ELECTRONICALLY CORRELATED MATERIALS AT AMBIENT AND EXTREME CONDITIONS**
$328,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: J. D. Thompson, (505) 667-6416

This coordinated program was aimed specifically at an in-depth description of the many-body ground state in correlated electron systems. This research examined heavy-electron compounds under extreme conditions of pressure, temperature, and magnetic field, thereby allowing unique insights into the correlated ground states.

Keywords: Heavy Electron Systems, Materials Under Extreme Conditions

379. **ORGANOMETALLIC CHEMICAL VAPOR DEPOSITION**
$248,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: D. C. Smith, (505) 667-2424

Most conventional metal halide based chemical vapor deposition processes take place at temperatures in excess of 800°C and produce corrosive gases (e.g., HCl, HF). Organometallic complexes as CVD precursors are a simple and powerful method for producing coatings at low temperatures, eliminating deleterious byproducts, and removing the halide from the process completely. In this effort, new routes to metal and metal carbide thin films from volatile organometallic precursors have been developed. Potential applications for these new low-temperature materials include: weapons diagnostics, oxidation protection coatings for polymers, barrier materials for use in nuclear fuels and high-temperature (>2000°C) environments, and coatings for solid propellants.

Keywords: Metal Thin Films, Metal Carbide Thin Films, Chemical Vapor Deposition

380. **POLYMER SORBENTS FOR HAZARDOUS METAL UPTAKE**
$164,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: B. Jorgensen, (505) 667-3619

Polymer sorbents with immobilized metal complexing agents are being developed for treatment of radioactive and mixed waste. The polymers are applicable to treatment of process streams, waste streams and environmental remediation. The polymers will remove hazardous metals and radionuclides from aqueous solutions. Two types of systems are being investigated. One of these is a water soluble polymer-supported extraction system for use in ultrafiltration technology and the other utilizes chelating resins. In each case, selective ligands are covalently bound to polymers and the polymers tested for metal ion uptake. Los Alamos is involved in the design, synthesis, and evaluation of actinide selective ligands in collaboration with several universities. Ligands developed in this program and other promising ligands are used in the polymer sorbents. The polymers are being tested on simulated waste mixtures and we hope to be able to test them on actual DOE radioactive waste.

Keywords: Metal Complexes, Radioactive Waste, Mixed Waste, Polymer Sorbents

381. **MICROSCOPIC MATERIALS MODELING: TEXTURES AND DYNAMICS**
$109,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: A. Bishop, (505) 667-6491

We applied analytical techniques developed in nonlinear science and simulation techniques using massively parallel computation to study textures and their dynamical consequences in areas of condensed matter and materials science. Specifically we have (1) implemented a Langevin MD code on the CM-2 that allows for study of large 2D Josephson junction arrays and 2D magnets; (2) simulated spiral surface growth in the presence of Frank-Read dislocation sources; (3) developed a nonlinear-nonlocal elasticity formalism for 2D martensitic materials; (4) discovered a new "glassy" relaxation response for large arrays of Josephson junctions in the presence of thermal noise and structural disorder; (5) used collective coordinate and MC-MD techniques to analyze the classical anisotropic Heisenberg model and relate dynamics of vortices to recent experiments.

Keywords: Textures, Condensed Matter, Materials Science, CM-2, Frank-Read Dislocations, Josephson Junctions, Heisenberg Model

382. **SURFACE MODIFICATION OF MATERIALS**
$315,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: M. Nastasi, (505) 667-7007

A combination of surface processing techniques, including reactive and non-reactive physical vapor deposition (PVD), ion implantation alloying, ion beam and excimer laser mixing, have been used to synthesize intermetallic,

ceramic, and composite coatings with amorphous and/or ultrafine-microstructures. The influence of synthesis variables on microstructural evolution and phase formation was evaluated using X-ray diffraction and transmission electron microscopy. Composition analysis was carried out using ion backscattering. The surface mechanical properties of these materials were evaluated for hardness and modulus using nanoindentation techniques and, in some instance, the friction and wear performance was also evaluated using a pin-on-disk tribometer.

Keywords: Physical Vapor Deposition, Ion Implantation, Ion Beam/Laser Mixing, Intermetallic Coatings, Ceramic Coatings, Composites

383. **INTEGRATION OF FUNDAMENTAL KNOWLEDGE IN PLASTICITY AND TEXTURES TO PROVIDE TECHNICAL TOOLS FOR MICROSCOPIC APPLICATIONS**
$290,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: U. F. Kocks, (505) 667-9323

The individual components of understanding that have been developed in basic research on mechanical properties are being integrated into a complete, coherent description of material behavior in plasticity. This involves the kinetics of flow and strain hardening, as well as texture development and the influence of textures on plastic anisotropy. Methods are established for determining the parameters required for applications of the model. User-friendly computer codes are maintained for the analysis of experimental textures, as well as for the prediction of current anisotropies on the basis of measured textures, and for the future development of texture and anisotropy during deformation through simulation of polycrystal plasticity. One aim is to foster development of a universal materials response package for incorporation into large engineering design codes for structures as well as processing. Conversely, these codes are used to derive properties of heterogeneous materials.

Keywords: Texture, Plastic Anisotropy, Plastic Deformation, Polycrystal Plasticity, Modeling

384. **HIGH RESOLUTION ELECTRON MICROSCOPY OF MATERIALS**
$350,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: T. E. Mitchell, (505) 667-0938

The high resolution electron microscopy (HREM) facility is based on a Philips CM30T microscope operating at 300 kV. Its point-to-point resolution of 1.9A makes it possible to obtain structure images of most materials at the atomic level. Image processing and enhancement procedures are being used to optimize the images obtained. Multi-slice image simulations on proposed structures are used to compare with experimental images and obtain information on atomic positions around defects such as dislocation and interfaces. HREM is being used on a wide range of materials applications. These include interfaces in semiconductor multilayers, grain boundaries in high temperature superconductors, twin boundaries in molybdenum disilicide, interfaces between silicon carbide and silicon nitride, and dislocations in refractory oxides.

Keywords: High Resolution Electron Microscopy, Materials at the Atomic Level, Molybdenum Disilicide, Silicon Carbide/Silicon Nitride Interfaces, Refractory Oxides

385. **NANO-FABRICATION**
$255,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: Robert Day, (505) 667-2957

This project combines theory and experiment to investigate the limits of nano-fabrication technology. We are primarily using molecular dynamics (MD) to simulate the actions and interaction of materials at the nanometer size. MD is used to study the stability of nanofeatures and to simulate nanomachining.

Keywords: Nano-fabrication, Molecular Dynamics, Nanomachining

386. **THIN FILM MICRO-ELECTROCHEMICAL SENSOR DEVELOPMENT**
$210,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: F. H. Garzon, (505) 667-6643

The objective of this project is the development of solid state microelectrochemical sensors that are applicable to the monitoring of hazardous gases such as: chlorine containing solvent vapors, sulfur dioxide, and halogen gases.

Keywords: Chemical Sensors, Chlorinated Hydrocarbons, Sulfur Oxides, Halogen Gases

387. **LIQUID CRYSTAL THERMOSETS**
$200,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
B. C. Benicewicz, (505) 665-0101

Designing composite materials at the nano-scale or molecular level is predicted to lead to mechanical properties several orders of magnitude greater than current materials. In the area of organic polymer composites, it has been shown that increases in properties are possible, but the usefulness of such materials is limited because of phase separation of the immiscible liquid crystal reinforcement and isotropic matrix components. This effort is a study of a new concept to make stable molecular composites using high performance liquid crystal polymers and newly developed liquid crystal thermoset matrices.

Keywords: Liquid Crystal Polymers

388. **NEUTRON AND RESONANT X-RAY SCATTERING BY MATERIALS**
$350,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
A. C. Lawson, (505) 667-8844

The techniques of pulsed neutron scattering and resonant X-ray diffraction are used to study materials such as actinides, f-electron ferromagnets and structural materials.

Keywords: Neutron Scattering, X-ray Scattering, Actinides, Ferromagnets

389. **STRUCTURAL AND ELECTRONIC COMPETITIONS IN LOW-DIMENSIONAL MATERIALS**
$360,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
B. I. Swanson, (505) 667-5814

This represents a combined theoretical and experimental study of the structural and electronic properties of low-dimensional electronic materials as they are tuned to the phase boundary region between different broken symmetry states (charge-density-and spin-density-wave, CDW and SDW). Within the CDW/SDW phase boundary region, competitions arise between the ground and local states (doping, photoinduced) that give rise to large changes in the transport (electrical) and optical properties. Work to date has focused on (1) developing new approaches to chemically tuning these materials through the phase boundary region, (2) studies (theory and experiment) of weak CDW and SDW materials, and (3) studies of mixed-halide materials, where the properties of the dominant species can be used to control the structure and electronics of the doped species. Key findings to date include (1) a new approach to tuning these materials through a structural "template" effect, (2) many-body modeling of species near the phase boundary region that shows evidence for CDW/SDW transitions and complex new structures, and (3) observation of the quenching of the Peierls distortion and the CDW in MX' segments of chains doped into a host MS lattice.

Keywords: Me Phase Boundary Tuning, Low-Dimensional Electronic Materials

390. **FUNDAMENTAL ASPECTS OF PHOTOELECTRON SPECTROSCOPY IN HIGHLY CORRELATED ELECTRONIC SYSTEMS**
$300,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
A. K. Arko, (505) 665-0758

Materials displaying strong electron-electron correlations continue to occupy condensed matter physicists, particularly in view of high T_c materials, where these correlations may be all important. Several variations of the Hubbard model are proposed as possible representations of this electronic structure. Photoelectron spectroscopy plays a major role in this research since it is one of the few experimental tools via which it is possible to observe the electronic structure directly without resorting to interpretation. We have performed numerous photoelectron spectroscopy tests on a large number of Ce- and Yb-based heavy fermions and compared the results to predictions of the model. Our single crystal data continue to indicate that the features usually identified as arising from the magnetic, or Kondo interaction, are much more logically described to first order as simple core levels.

Keywords: Photoemission Spectroscopy, Electronic Correlations

391. **DEVELOPMENT OF HIGH STRENGTH HIGH CONDUCTIVITY MATERIALS FOR HIGH MAGNETIC FIELD DEVICES**
$100,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
F. M. Mueller, (505) 667-9244

The project will cover the fabrication analysis and design of high strength high conductivity materials for pulsed magnet applications of relevance to NHMFL. New methods of fabrication will be considered based on the use of rapid solidification and cryogenic forming. An analysis of the

materials will be conducted based on measurement of mechanical properties, characterization of the structure by SEM and TEM methods and measurement of the ratio of the electrical conductivity at 293K and 77K as a function of the material's thermal-mechanical history. Attempts will be made to link the results of the study directly to the needs of NHMFL in terms of both magnetic coil design and optimization of relevant fabrication methods.

Keywords: Conductive Materials, Magnetic Coil Designs

392. **LOW TEMPERATURE STM FOR STRUCTURAL AND SPECTROSCOPIC STUDIES OF HIGH TEMPERATURE SUPERCONDUCTORS AND OTHER ELECTRONIC MATERIALS**
$50,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: M. Hawley, (505) 665-3600

The STM is a powerful probe of the local density of states in the study of electronic materials. The extension of this capability to low temperatures creates an opportunity to apply this technique to such studies as phase transitions in low dimensional electronic materials and in superconductors, i.e., I-V gap measurements and vortex lattices. To this end, this program includes the design and construction of a variable low temperature STM for the study of these materials. Where possible, we will explore the utility of this technique in the study of changes in morphology of structural materials with lower temperature applications and to the fabrication of nanoscale features.

Keywords: Scanning Tunneling Microscope, Electronic Materials, Low Temperature Scanning

393. **MATERIALS WITH FINE MICROSTRUCTURES**
$365,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: R. B. Schwarz, (505) 667-8454

The refinement of the microstructure of multiphase alloys can lead to significant enhancements in the mechanical properties of engineered materials. One synthesis route for such materials is the consolidation of powders with fine microstructures. This program addresses both the problem of synthesizing powders with fine microstructures and the problem of consolidating these powders while preserving their fine microstructure.

Keywords: Multiphase Alloys, Microstructure, Powder Consolidation

394. **ION BEAM MATERIALS RESEARCH**
$330,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: C. J. Maggiore, (505) 667-6133

The synthesis of any new material cannot proceed efficiently without the quantitative characterization of the composition and structure of the material actually fabricated. The use of MeV ions is a well understood means of quantitative analysis and is routinely available at the IBML (Ion Beam Materials Laboratory). However, the continued development of new materials with better defined structure and composition on a finer scale has placed more stringent requirements on existing analytical methods. The objective of this program is to extend the analytical range and applicability of the IBML to the classes of new synthetic materials of current technological interest. Samples will be prepared by a variety of collaborators that are suitable for studying the fundamental limitations of multiple straggling on depth resolution using ion beams, improving sensitivity limits for light elements in complex samples using prompt and delayed nuclear reaction analysis, and bulk detection of hydrogen.

Keywords: Ion Beam Characterization

395. **TEXTURE STUDIES OF HIGHLY DEFORMED COMPOSITE MATERIALS**
$192,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: A. C. Larson, (505) 667-2942

Recently scientists have become interested in creating composite materials, such as high Tc-superconductors encased in silver wire and then deformed to prepare a tape, aluminum with SiC whiskers embedded in the aluminum matrix and copper metal containing tungsten wires. These composite materials are an effort to prepare materials displaying an optimal combination of the properties of the component materials. It is important to recognize that, in the deformation of two-phase systems, two processes become of importance: (a) the development of accommodation strain or arrays of geometrically necessary dislocations around the particles of the more rigid phase and (b) a change in the patterns of the flow in each phase due to the presence of the other phase. The occurrence of these processes is dependent on the relative fractions of the phases. We propose to study the relationships among the phases present in a composite by

examination of the texture or orientation distribution of the crystallites in each phase.

Keywords: Silicon Carbide Whisker Reinforced Aluminum, Tungsten Wire Reinforced Copper, Two Phase Deformation

396. **PRESSURE DEPENDENCY OF THE STRUCTURE OF HIGH EXPLOSIVES: NITROMETHANE**
$192,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: R. B. VonDreele, (505) 667-3630

This program examines the structural changes as a function of pressure for nitromethane and correlates them with the pressure dependence of solid state ionization processes proposed as an explosion front propagation mechanism.

Keywords: Nitromethane, Pressure Dependencies, Explosive Front Propagation Mechanisms

397. **NEUTRON REFLECTION STUDIES OF THIN FILM AND MULTILAYER STRUCTURES**
$300,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: M. R. Fitzsimmons, (505) 665-4045

The purpose of this research program is to understand magnetism in thin film and multilayer structures using polarized neutron reflection (PNR). In order to obtain meaningful measurements of the magnetic structures and properties of surfaces and interfaces, the capability to manufacture thin films and multilayers, while PNR measurements are made, is essential. Such a capability-a first for a neutron source-will be developed. Topics to be explored by this research program are: two-dimensional magnetism, the kinetics of diffusion within multilayers, diffusion-induced changes of the magnetic properties of multilayers, the correlation between the magnetic properties of surfaces and interfaces with their roughness, and the design of improved super-mirrors for neutron applications.

Keywords: Magnetic Properties of Thin Films, Polarized Neutron Diffusion in Multilayers

398. **NEUTRON REFLECTIVITY STUDIES OF IN SITU CORROSION OF METAL SURFACES**
$145,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: G. S. Smith, (505) 665-2842

Corrosion of metallic surfaces have been studied for many years by several techniques. These studies have looked at the problem of corrosion both as a problem to be eradicated and as a useful end to the electroplating process. Never before has anyone been able to look at the microscopic details of composition as well as surface roughness at the metal-electrolyte interface. This program uses neutron reflectometry to study these features.

Keywords: Corrosion, Neutron Reflectometry

399. **THE DYNAMICS OF AMORPHOUS MATERIALS**
$330,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: R. A. Robinson, (505) 667-3626

This research program studies the vibrational and magnetic dynamics of amorphous materials, using inelastic neutron scattering. While atomic and magnetic fluctuations are well understood as collective excitations (e.g., phonons, magnons) in single crystals, much less is understood in amorphous materials. The materials to be studied include silica, porous silica aerogels, a metallic glass and metglas.

Keywords: Vibration Dynamics, Magnetic Dynamics, Silica, Silica Aerogels, Metallic Glasses

400. **ADVANCED MATERIAL SCIENCE ALGORITHMS FOR SUPERCOMPUTER ARCHITECTURES**
$75,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: J. E. Gubernatis, (505) 667-6727

This project is concerned with exploiting the potential new computer architectures offer to improving the understanding and modeling of material properties and behavior through computer simulation. The focus is on developing the simulation ability to study flux line dynamics, noise, melting, and pinning in London and Ginzburg-Landau phenomenological models of thin films on high temperature superconducting materials. The

emphasis of the program is also on parallizing the world-line quantum Monte Carlo method and developing procedures to extract dynamical information from imaginary-time quantum Monte Carlo data.

Keywords: High Temperature Superconducting Materials, London Phenomenological Models, Ginzburg-Landau Phenomenological Models

401. **METAL VAPOR SYNTHESIS IN ORGANOMETALLIC CHEMISTRY**
$235,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: J. G. Watkin, (505) 667-4546

This program will employ the rare synthetic technique of metal vapor synthesis (MVS) to prepare a series of organometallic complexes of middle- and late-transition metals and lanthanides. Applications include catalytic processes and/or organic synthesis. The technique of metal vapor synthesis has been employed to prepare many examples of low-valent early transition metal complexes which have been shown to exhibit high reactivity, but the technique has rarely been applied to the later transition metals such as Rh, Ir, Pd, Pt and the lanthanides.

Keywords: Metal Vapor Synthesis, Lanthanides

402. **SEPARATION CHEMISTRY OF TOXIC METALS**
$250,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: P. H. Smith, (505) 667-1604

The goal of this research is to develop a new class of chelators for toxic metals which have the capacity to bind two species and where the binding of one substrate affects the binding of the second. In the process we hope to gain a fundamental understanding of the key parameters which govern toxic metal ion selective binding as it relates to separations chemistry. We will synthesize and evaluate a class of chelators which add a new dimension to coordination chemistry, namely cooperative/antagonistic binding. The chemistry involves the development and synthesis of ditopical receptors which contain two binding sites in close proximity to each other. In systems with cation and anion sites, the simultaneous binding of both a cation and an anion can enhance the overall binding constants relative to either one binding alone.

Keywords: Cooperative/Antagonistic Binding Sites, Chelates, Ditopical Receptors

403. **POLYMERS FOR INTEGRATED OPTICAL INTERCONNECTS**
$266,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: B. Laurich, (505) 665-0333

The recent discovery of electroluminescent polymers opens up, for the first time, the possibility of using optical interconnects for conventional silicon integrated circuits. If this capability can be realized, it will have a tremendous impact on the architecture and performance of the complex computing and communications systems.

Keywords: Electroluminescent Polymers, Integrated Optical Interconnects

404. **HIGH TEMPERATURE MATERIALS SYNTHESIS WITHOUT HEAT: OXIDE LAYER GROWTH ON ELECTRONIC MATERIALS USING HIGH KINETIC ENERGY ATOMIC SPECIES**
$164,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: M. A. Hoffbauer, (505) 667-4878

This research program examines high temperature materials synthesis using high kinetic energy atomic species instead of heat. Emphasis is being placed on the direct growth of oxide and nitride insulating layers on compound semiconducting electronic materials such as GaAs where we have already shown the unprecedented formation of oxide layers that are thick, uniform, and of extremely high quality. Research into this novel material synthesis process with the aim of producing and demonstrating device-quality oxide layers is being emphasized. Application of this materials synthesis technology to space-based manufacturing technology is also being pursued.

Keywords: Ceramic Oxides, Ceramic Nitrides, Insulating Layers, KE Atomic Heating

405. **DYNAMIC DEFORMATION OF ADVANCED MATERIALS**
$855,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: G. T. Gray, (505) 667-5452

Composites, metal or ceramic matrix, and advanced materials, such as intermetallics, are receiving increasing attention due to their higher specific strengths, stiffness, and high temperature properties. Advanced composites also allow other physical properties besides mechanical properties to be custom tailored to specific applications.

Increased utilization of these material classes under dynamic loading conditions requires an understanding of the relationship between high-rate/shock-wave response as a function of microstructure if predictive material behavior capabilities are to be attained. This program is a multidisciplinary effort to investigate the influence of microstructure, anisotropy, orientation, and structural ordering on the high-strain-rate and shock-wave deformation behavior of advanced composites and intermetallics. The long-term objective is to provide high quality experimental measurements on advanced materials to facilitate the development of predictive computational models.

Keywords: High-Strain Rate Deformation, Shock-Wave Deformation, Composites, Intermetallics

406. **STRAIN MEASUREMENTS IN INDIVIDUAL PHASES OF MULTI-PHASE MATERIALS**
$130,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: J. A. Goldstone, (505) 667-3629

Employment of metal matrix and ceramic composites in high-technology aerospace applications or as lighter (more economic) material in the auto industry requires the development of analytical methods capable of predicting the durability, debonding, and damage tolerance during the mechanical and thermal loads expected during service. Neutron diffraction has been used to measure residual stress in composites, steels, and compacted powders. We wish to extend our capability by acquiring a stress rig with a furnace to make in situ measurements of material response. This will permit measurements on technologically important materials under conditions close to service. Preliminary studies will address an Al/TiC composite (under consideration for automotive use) and $MoSi_2$.

Keywords: Neutron Diffraction, Aluminum/Titanium Carbide Composites, Molybdenum Disilicide Composites

407. **ARTIFICIALLY STRUCTURED NONLINEAR OPTIC AND ELECTRO-OPTIC MATERIALS**
$465,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: B. I. Swanson, (505) 667-5814

New artificially structured materials that are optimized for nonlinear optic (NLO) and electro-optic applications will be synthesized, characterized, and modeled. Materials based on two new synthetic strategies will be pursued. Chromophores with optical absorptions tuned to the red and near-IR portion of the spectrum will be directly attached to optical surfaces through the use of covalent bonding of self-assembled (CBSA) mono- and multilayers. The second strategy is based on the construction of single hetero-junctions or multiple hetero-junctions in superlattice materials where charge separation across the junctions results in optimal NLO and electro-optic properties. The overall goal is to further develop these two synthetic approaches through a combined synthesis, characterization, and theory effort where materials modeling, benchmarked by observed physical properties, is used to guide rational synthesis of advanced materials.

Keywords: Nonlinear Optic Materials, Electro-Optic Materials, Superlattice Materials

408. **STRUCTURAL PHASE TRANSITIONS IN NON-STOICHIOMETRIC OXIDES**
$275,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: A. Migliori, (505) 667-2515

Structural phase transitions (SPT) have profound effects on mechanical, magnetic, and electronic properties. In Stoichiometric compounds, SPTs are well understood and produce the magnetism in ferrites and the ferroelectricity in piezoelectric oxides that make these materials so important. However, for non-stoichiometric compounds, the situation is very far from clear, and the puzzles are not merely academic. For example, the high T_c perovskite $La_{2-x}Sr_xCuO_4$ undergoes a second-order SPT from a tetragonal to an orthorhombic structure upon cooling through $T_s(x)$. As T_s is approached from either direction, one shear modulus collapses, making the material mechanically partially unstable, a non-trivial consequence for applications. The surprise is that this collapse begins 100K above T_s, not at 2K predicted by the best theoretical approach. Resonant Ultrasound Spectroscopic (RUS) studies of this and other SPTs reveal additional and subtle problems with current theory, not observed with any other experimental problem. Lack of just this sort of observation has stymied the theory of SPTs in heavily doped crystals because a simple observation of modulus collapse cannot distinguish between several competing possibilities. An understanding of the effects of doping on material properties near SPTs is of extreme fundamental interest and is crucial for a very broad spectrum of applications; recent observations by us suggest that only LANL's unique RUS capability can provide the necessary clues.

Keywords: Resonant Ultrasound Spectroscopy, Structural Phase Transitions

409. **STRONGLY CORRELATED ELECTRONIC MATERIALS**
$495,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
K. S. Bedell, (505) 665-0478

New, novel materials have a number of extraordinary and often unexpected properties and, it is likely, they will play a major role in the high-technology electronic materials of the future. To better design materials for specific applications it is necessary to understand the microscopic origins of their novel physical characteristics. To relate the microscopic models of these strongly correlated systems to specific materials properties requires the extension of and the development of new many-body techniques. This program provides the basic science component for a number of new initiatives that include the Presidential initiative in materials science, the Advanced Computing Laboratory (ACL), the use of novel electronic materials for device applications, the National High Magnetic Field Laboratory (NHMFL), the UC Los Alamos INCOR program in high temperature superconductivity (HTS), and the Program in Correlated Electron Theory.

Keywords: High-Temperature Electronic Materials, Electronic Correlations

410. **PLASMA IMMERSION ION IMPLANTATION FOR SEMICONDUCTOR FILM GROWTH**
$261,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
M. Tuszewski, (505) 667-3566

An interdisciplinary team of plasma and semiconductor physicists will develop a novel plasma implanter for thin film growth on semiconductors with unprecedented control. The scientific objectives of this project are: (1) construction of a compact, inexpensive, and high-throughput implanter based on an inductive plasma source and on e plasma immersion ion implantation (PIII) technique; (2) extension of the PIII technique to higher frequencies, lower voltages, and higher dose rates; (3) characterization, optimization, and control of the plasma species concentrations and impurities; (4) generation of semiconductor dielectrics and alloys for new electronics device technologies.

Keywords: Plasma Ion Implantation, Semiconducting Materials

411. **ANALYSIS OF STRUCTURE AND ORIENTATION OF ADSORBED POLYMER IN SOLUTION SUBJECT TO DYNAMIC SHEAR STRESS**
$172,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
S. Baker, (505) 667-6069

Polymer based separation techniques rely on the ability of a binding portion of the polymer to interact with a specific molecule in a solution flowing past the polymer. The location of the binding site within or out of the entangled polymer chains is thus crucial to the effectiveness of these methods. For this reason, the details of flow induced deformation of the polymer chains is important in such applications as exclusion chromatography, waste water treatment, ultrafiltration, enhanced oil recovery and microbial adhesion. Few techniques exist to examine the structure and orientation of polymeric materials, and even fewer to examine systems in a dynamic fluid flow. The goal of this program is to understand the molecular structure and orientation of adsorbed polymers with and without active binding ligands as a function of solvent shear rate, solvent ower, polymer molecular weight, surface polymer coverage, and heterogeneity of the surface polymer chains by neutron reflectometry in a newly Designed shear cell. Geometrical effects on binding of molecules in the flow will also be studied subject to the same parameters.

Keywords: Polymer Molecules, Neutron Reflectometry, Flow Induced Deformation

412. **DEVELOPMENT OF PAIR DISTRIBUTION FUNCTION ANALYSIS OF MESOSTRUCTURAL DETAILS IN SINGLE CRYSTAL PEROVSKITES AND NANOCRYSTALLINE MATERIALS**
$170,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
G. H. Kwei, (505) 667-8840

It has become increasingly evident that structural coherence in the CuO_2 planes of high-Tc superconducting (HTSC) materials over some intermediate length scale (in the nanometer range) is important to superconductivity. Significant progress has been made in understanding these structural instabilities using pair distribution function analysis of powder diffraction data. However, PDF diffraction data on single crystals is required, both because of the greater amount of information in the latter and because of the much greater sample quality that is available in single crystals. The goal of this program is to develop analysis techniques for obtaining PDF's from single crystal diffraction data and to use these techniques to

study structural instabilities and structural coherence in HTSC and other interesting materials. PDF techniques are also planned for studying mesostructural features in nanocrystalline materials.

Keywords: Powder Diffraction Analysis, High Temperature Superconductors, Mesostructural Nanocrystals

413. **NEUTRON SCATTERING AS A PROBE OF THE STRUCTURE OF LIQUID CRYSTAL POLYMER-REINFORCED COMPOSITE MATERIALS**
$180,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: R. P. Hjelm, (505) 665-2372

The goal of this program is to obtain nanoscale and molecular level information on the mechanism of reinforcement 9n crystal polymer-reinforced composites, and to realize the production of molecularly-reinforced LCP composites. Small-angle neutron scattering methods are proposed to study the structures on length scales ranging from 10-1000 Å. The goal of the small-angle scattering measurements is to understand the morphology of separation of the reinforcing and matrix phases as a function of composition, mixing, temperature and other process conditions. This information will be correlated with mechanical properties to achieve a better understanding of the molecular mechanism of reinforcement.

Keywords: Small-Angle Neutron Scattering, Polymer Composites

414. **STRAIN MEASUREMENTS IN INDIVIDUAL PHASES OF MULTI-PHASED MATERIALS DURING THERMO-MECHANICAL LOADING: LANSCE NEUTRON SCATTERING EXPERIMENT SUPPORT**
$318,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: J. A. Goldstone, (505) 667-3629

Employment of metal matrix and ceramic composites in high-technology aerospace applications or as lighter (more economic) material, in the auto industry requires the development of analytical methods capable of predicting the durability, debonding, and damage tolerance during the mechanical and thermal loads expected during service. Neutron diffraction has been used to measure residual stress in composites, steels and compacted powders. We wish to extend our capability by acquiring a stress rig with a furnace to make in situ measurements of material response. This will permit measurements on technologically important materials under conditions close to service. Preliminary studies will address an Al/TiC composite (under consideration for automotive use) and $MoSi_2$.

Keywords: Neutron Diffraction, Metal Matrix Composites, Ceramic Matrix Composites

415. **A NEW APPROACH TO TEXTURE MEASUREMENTS: ODF DETERMINATION BY RIETVELD REFINEMENT**
$73,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: R. B. VonDreele, (505) 667-3630

This program centers on the development of the experimental procedures and the mathematical treatment needed to produce an orientation distribution function (ODF) directly from full diffraction patterns from a sample in a limited number of orientations.

Keywords: Texture Measurement, Orientation Distribution Function, Diffraction Patterns

416. **APPLICATIONS OF FULLERENES IN NUCLEAR TECHNOLOGY**
$360,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact: D. K. Veirs, (505) 667-9291

The major focus of our research efforts is in the use of fullerene-based materials in the solution to problems in the nuclear research and industry. Fullerene encapsulation of nuclear waste is of interest in the storage of high-level nuclear waste. Fullerene-encapsulated uranium or plutonium may be very stable with respect to the environment and may provide a safe and efficient way of disposing of nuclear waste. The metal-in-fullerene aspect or metal-doped fullerene compounds in conjunction with the high thermal stability and low density of fullerene suggests the fabrication of efficient, high-yield targets for the production of radioactive beams. It is likely that a target composed fullerene, upon proton-induced fission or spallation of the uranium, will allow the efficient release of the fission or spallation products for the purpose of producing radioactive nuclear beams. We propose to explore the production of actinide fullerides and to develop the relevant technology to generate and separate them for these purposes.

Keywords: Fullerenes, Encapsulation, Nuclear Waste, Uranium, Plutonium

417. **CERAMIC OXIDE FOAMS FOR SEPARATION**
$400,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
P. C. Apen, (505) 665-7513

Ceramic oxide foams and novel foam structures are playing an important role in environmental R&D, specifically in the areas of chemical separations and filtration for removal of heavy metals and particulates from contaminated waste streams and effluent. This program focusses on the investigation of virgin oxide and surface-modified oxide foams in environmental remediation applications. Processes for the preparation and modification of porous ceramic structures will be developed and the products characterized for functionality in the separation of heavy metal and toxic particulates from waste streams.

Keywords: Silica Foams, Silica Sol-Gels, Heavy Metal Ligands, Metal Ion Chelating Agents

418. **MATERIALS MODELING PROJECT**
$125,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
R. LeSar, (505) 665-0420

This program involves the modeling of laser-assisted deposition processes with an emphasis on laser/solid interactions, plasma chemistry and dynamics, nucleation and growth, and the theoretical design of novel materials. The modeling will also involve analytical studies of strain-induced diffusion along specific interfaces and Monte Carlo studies of diffusion in polycrystalline materials. The goal of the program is to link this work with a micromechanical fracture model.

Keywords: Laser-Assisted Deposition Processes, Micromechanical Fracture Models, Plasma Chemistry

419. **SYNTHESIS AND OPTICAL CHARACTERIZATION OF NOVEL FULLERENE-BASED COMPOSITES**
$50,000
DOE Contact: M. J. Katz, (202) 586-5799
LANL (Contract No. W-7405-ENG-36) Contact:
J. M. Robinson, (505) 665-4834

This program takes an interdisciplinary approach to develop and study a novel family of fullerene-based organic and inorganic composites for applications as photodiodes and photovoltaic devices. The emphasis of the program is on "proof of principle" for the synthesis of new composite materials which will guide further synthetic refinements. A novel "host-guest" chemistry will result in two new classes of materials. The first class utilizes sol-gel chemistry to incorporate fullerenes into optically transparent hosts that are processable into thick glass monoliths or thin film waveguides. The principal role of the host is to protect the fullerene guests from environmental degradation, and to provide a low loss transparent medium for light transmission. The second class of materials is based on fullerene/conjugated polymer composites.

Keywords: Fullerene Composites, Photodiodes, Photovoltaic Devices, Sol-Gels

TECHNOLOGY TRANSFER INITIATIVE

420. **A PILOT PROGRAM: CHEMICAL VAPOR DEPOSITION OF DIAMOND IN A FLUIDIZED-BED FOR CUTTING TOOL AND TRIBOLOGICAL APPLICATIONS**
$250,000
DOE Contact: W. P. Chernock (202) 586-7590
LANL (Contract No. W-7405-ENG-36) Contact:
David Carroll, (505) 667-2145

A program to develop and commercialize a process to generate high-quality diamond coatings for machine tools.

Keywords: Diamond Coatings, Chemical Vapor Deposition, Cutting Tools, Tribology

421. **ADVANCED BERYLLIUM PROCESSING**
$632,000
DOE Contact: W. P. Chernock (202) 586-7590
LANL (Contract No. W-7405-ENG-36) Contact:
Loren Jacobson, (505) 667-5151

A program to produce beryllium powders and rolled beryllium sheet using improved manufacturing techniques that minimize worker exposure and reduce the environmental consequences of beryllium processing.

Keywords: Beryllium Processing, Beryllium Alloy Processing, Centrifugal Atomization

422. **AUTOMATED PULSED LASER DEPOSITION SYSTEM**
$130,000
DOE Contact: W. P. Chernock (202) 586-7590
LANL (Contract No. W-7405-ENG-36) Contact:
Ross Muenchausen, (505) 665-4949

A program to design an automated pulsed laser deposition system to deposit high-temperature superconducting thin films.

Keywords: Pulsed-Laser-Deposition, High-Temperature Superconducting Films

423. **PLASMA SOURCE ION IMPLANTATION FOR THE AUTOMOTIVE INDUSTRY**
$1,326,000
DOE Contact: W. P. Chernock (202) 586-7590
LANL (Contract No. W-7405-ENG-36) Contact:
Donald Rej (505) 665-1883

A program to develop a production-scale plasma-source ion implantation system for improving the surface properties of auto parts.

Keywords: Plasmas, Ion Implantation, Tool Hardening

424. **PROCESSING MODELING AND CONTROL FOR U.S. STEEL INDUSTRY**
$1,195,000
DOE Contact: W. P. Chernock (202) 586-7590
LANL (Contract No. W-7405-ENG-36) Contact:
Brian Lally, (505) 667-9954

A program to develop new process models and control systems for the U.S. Steel Industry.

Keywords: Steel, Electric-Arc-Furnace, Scrap Steels